Welcome to STN International! Enter x:x

LOGINID:sssptau121bd

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

09/891026

Welcome to STN International Web Page URLs for STN Seminar Schedule - N. America NEWS Jan 25 BLAST(R) searching in REGISTRY available in STN on the Web NEWS NEWS 3 Jan 25 Searching with the P indicator for Preparations NEWS 4 Jan 29 FSTA has been reloaded and moves to weekly updates NEWS 5 Feb 01 DKILIT now produced by FIZ Karlsruhe and has a new update frequency NEWS Feb 19 Access via Tymnet and SprintNet Eliminated Effective 3/31/02 NEWS 7 Mar 08 Gene Names now available in BIOSIS NEWS 8 Mar 22 TOXLIT no longer available NEWS 9 Mar 22 TRCTHERMO no longer available NEWS 10 Mar 28 US Provisional Priorities searched with P in CA/CAplus and USPATFULL NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002 NEWS HOURS STN Operating Hours Plus Help Desk Availability General Internet Information NEWS INTER NEWS LOGIN Welcome Banner and News Items NEWS PHONE Direct Dial and Telecommunication Network Access to STN NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 13:41:24 ON 28 MAR 2002

#### => fil regh

\*\*\* YOU HAVE NEW MAIL \*\*\*

'REGH' IS NOT A VALID FILE NAME SESSION CONTINUES IN FILE 'HOME'

Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

## => fil req

FILE 'REGISTRY' ENTERED AT 13:42:07 ON 28 MAR 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS) STRUCTURE FILE UPDATES: 26 MAR 2002 HIGHEST RN 402912-59-8 DICTIONARY FILE UPDATES: 26 MAR 2002 HIGHEST RN 402912-59-8

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

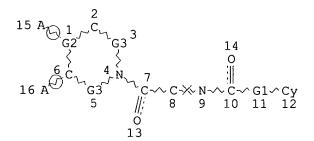
Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

\*\*\* YOU HAVE NEW MAIL \*\*\*

'.REGISTRY' IS DEFAULT FORMAT FOR 'REGISTRY' FILE

=> d sia L1 HAS NO ANSWERS L1 STR

REP G1 = (0-2) C



VAR G2=N/C REP G3=(0-2) CH NODE ATTRIBUTES: NSPEC IS RC 8 NSPEC IS RC ΑT 9 NSPEC IS R AT15 NSPEC IS R ΑT 16 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 16

## STEREO ATTRIBUTES: NONE

=> s 11 SAMPLE SEARCH INITIATED 13:58:09 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 14801 TO ITERATE

6.8% PROCESSED 1000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 288749 TO 303291 PROJECTED ANSWERS: 2231 TO 3689

L2 10 SEA SSS SAM L1

=> d scan

L2 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-tryptophyl-N-[1-[(3,4-dihydro-2(1H)-isoquinolinyl)carbonyl]-3-oxo-3-(phenylmethoxy)propyl]-3-(2-naphthalenyl)-, (S)- (9CI)

10 ANSWERS

MF C49 H51 N5 O7

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L2 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-[2-(3,4-dihydro-6,7-dimethoxy-1-methyl-2(1H)-isoquinolinyl)-2-oxoethyl]-4-(1,1-dimethylethyl)-N-ethyl- (9CI)

MF C27 H36 N2 O4

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, 3-bromo-N-[2-(3,4-dihydro-1-methyl-2(1H)-isoquinolinyl)-2oxoethyl]-N-(3-methylbutyl)- (9CI)

MF C24 H29 Br N2 O2

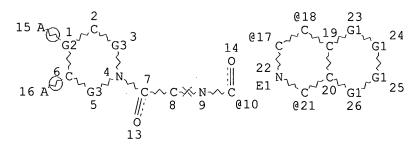
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> str l1 => d sia

L3 HAS NO ANSWERS

L3 STI



VAR G1=C/O/S/N

VAR G2=N/C

REP G3=(0-2) CH

VPA 10-18/17/21 U

NODE ATTRIBUTES:

HCOUNT IS E1 AT 22

NSPEC IS RC AT 8

NSPEC IS RC AT 9

NSPEC IS R AT 15 NSPEC IS R AT 16

NSPEC IS R AT 16 DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

=> s 13 SAMPLE SEARCH INITIATED 14:09:43 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 3655 TO ITERATE

27.4% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 69477 TO 7672

PROJECTED ITERATIONS: 69477 TO 76723 PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L3

=> s 13 ful FULL SEARCH INITIATED 14:10:28 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 72169 TO ITERATE

100.0% PROCESSED 72169 ITERATIONS 25 ANSWERS SEARCH TIME: 00.00.05

0 ANSWERS

L5 25 SEA SSS FUL L3

=> d tot reg can

1 RN 384345-35-1 REGISTRY

REFERENCE 1: 136:69824

2 RN 384345-34-0 REGISTRY

REFERENCE 1: 136:69824

3 RN 384345-33-9 REGISTRY

REFERENCE 1: 136:69824

4 RN 384345-32-8 REGISTRY

REFERENCE 1: 136:69824

5 RN 384345-31-7 REGISTRY

REFERENCE 1: 136:69824

6 RN 384345-30-6 REGISTRY

REFERENCE 1: 136:69824

7 RN 384345-29-3 REGISTRY

REFERENCE 1: 136:69824

8 RN 384345-28-2 REGISTRY

REFERENCE 1: 136:69824

9 RN 384345-27-1 REGISTRY

REFERENCE 1: 136:69824

10 RN 384345-26-0 REGISTRY

REFERENCE 1: 136:69824

11 RN 384345-25-9 REGISTRY

REFERENCE 1: 136:69824

12 RN 384345-24-8 REGISTRY

REFERENCE 1: 136:69824

13 RN 384345-23-7 REGISTRY

REFERENCE 1: 136:69824

•				
14	RN		384345-22-6	REGISTRY
REFERENCE 15	1: RN	136:69824	384345-21-5	REGISTRY
REFERENCE 16	1: RN	136:69824	1 384345-17-9	REGISTRY
REFERENCE 17	1: RN	136:69824	1 384345-16-8	REGISTRY
REFERENCE 18	1: RN	136:69824	384345-14-6	REGISTRY
REFERENCE 19	1: RN	136:69824	384345-11-3	REGISTRY
REFERENCE 20	1: RN	136:69824	1 384345-08-8	REGISTRY
REFERENCE 21 136:15253	1: RN	136:69824	1 378741-82-3	REGISTRY
REFERENCE 22	1: RN	136:15253	3 378741 <b>-</b> 76-5	REGISTRY
REFERENCE 23	1: RN	136:15253	3 176714-38-8	REGISTRY
REFERENCE 24	1: RN	124:33332	25 176714-37-7	REGISTRY

# => d 1 21 24 26 ide

RN

REFERENCE 1: 124:306933

REFERENCE

25

25 ANSWERS ARE AVAILABLE. SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE The answer numbers requested are not in the answer set. ENTER ANSWER NUMBER OR RANGE (1):1 21 24 25

176177-87-0 REGISTRY

L5 ANSWER 1 OF 25 REGISTRY COPYRIGHT 2002 ACS

1: 124:333325

- RN 384345-35-1 REGISTRY
- CN 3-Isoquinolinecarboxamide, N-[(1R)-1-[(4-chlorophenyl)methyl]-2-[8a-[(4-fluorophenyl)methyl]hexahydro-2-methyl-1,3-dioxoimidazo[1,5-a]pyrazin-7(1H)-yl]-2-oxoethyl]-1,2,3,4-tetrahydro-, (3S)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C33 H33 C1 F N5 O4
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 1 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)
- ANSWER 21 OF 25 REGISTRY COPYRIGHT 2002 ACS 378741-82-3 REGISTRY L5
- RN
- CN 3-Isoquinolinecarboxamide, N-[(1R)-1-[(4-chlorophenyl)methyl]-2-[2,3,3a,4,6,7-hexahydro-2-methyl-3-oxo-3a-(phenylmethyl)-5H-pyrazolo[4,3-c]pyridin-5-yl]-2-oxoethyl]-1,2,3,4-tetrahydro-, (3R)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)
- STEREOSEARCH FS
- C33 H34 C1 N5 O3 . C2 H F3 O2 MF
- SR CA
- LCSTN Files: CA, CAPLUS, USPATFULL

CM1

378741-76-5 CRN CMF C33 H34 C1 N5 O3

Absolute stereochemistry.

CM2

CRN 76-05-1 CMF C2 H F3 O2

# 1 REFERENCES IN FILE CA (1967 TO DATE) 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L5 ANSWER 24 OF 25 REGISTRY COPYRIGHT 2002 ACS

RN 176714-37-7 REGISTRY

CN 3-Isoquinolinecarboxamide, 1,2,3,4-tetrahydro-2-[[4-hydroxy-1-[(1,2,3,4-tetrahydro-3-isoquinolinyl)carbonyl]-2-pyrrolidinyl]carbonyl]-N-methyl-N-(phenylmethyl)-, [2S-[1(R\*),2.alpha.(R\*),4.beta.]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C33 H36 N4 O4

SR CA

LC STN Files: CA, CAPLUS

# Absolute stereochemistry.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 1 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)
- L5 ANSWER 25 OF 25 REGISTRY COPYRIGHT 2002 ACS
- RN 176177-87-0 REGISTRY
- CN L-Arginine, N-[(1,2,3,4-tetrahydro-3-isoquinolinyl)carbonyl]-L-seryl-D-1,2,3,4-tetrahydro-3-isoquinolinecarbonyl-L-(2.alpha.,3a.beta.,7a.beta.)-octahydro-1H-indole-2-carbonyl-, (R)- (9CI) (CA INDEX NAME)
- FS PROTEIN SEQUENCE; STEREOSEARCH
- MF C38 H50 N8 O7
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

- 1 REFERENCES IN FILE CA (1967 TO DATE) 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)
- => fil stnguide FILE 'STNGUIDE' ENTERED AT 14:12:08 ON 28 MAR 2002 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Mar 22, 2002 (20020322/UP).

=> fi reg

FI IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> fil reg FILE 'REGISTRY' ENTERED AT 14:15:41 ON 28 MAR 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 26 MAR 2002 HIGHEST RN 402912-59-8 DICTIONARY FILE UPDATES: 26 MAR 2002 HIGHEST RN 402912-59-8

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number

or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

\*\*\* YOU HAVE NEW MAIL \*\*\*

'.REGISTRY' IS DEFAULT FORMAT FOR 'REGISTRY' FILE

=> d 20 22 sub bib abs

L5 ANSWER 20 OF 25 REGISTRY COPYRIGHT 2002 ACS

RN 384345-08-8 REGISTRY

CN 3-Isoquinolinecarboxamide, N-[(1R)-1-[(4-chlorophenyl)methyl]-2-[hexahydro-1,3-dioxo-8a-(2-pyridinylmethyl)-2-(2,2,2-trifluoroethyl)imidazo[1,5-a]pyrazin-7(1H)-yl]-2-oxoethyl]-1,2,3,4-tetrahydro-, hydrochloride, (3S)-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C33 H32 Cl F3 N6 O4 .  $\times$  Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

•x HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

## REFERENCE 1

AN 136:69824 CA

TI Preparation of heterocycle compounds as melanocortin receptor ligands

IN Carpino, Philip Albert; Cole, Bridget McCarthy; Morgan, Bradley Paul

PA Pfizer Products Inc., USA

SO PCT Int. Appl., 108 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.	CNT 1															
	PATENT	NO.	KI	ND	DATE			A	PPLI	CATI	ON NO	). I	DATE			
								_								
ΡI	PI WO 2002000654		A	A1 20020103			WO 2001-IB995					20010531				
	W:	AE, A	G, AL,	ΑM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		CO, C	R, CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM, H	R, HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,
		LS, L	r, Lu,	LV,	ΜA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	ΝZ,	PL,	PT,
		RO, R	U, SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,
		UZ, V	N, YU,	ZA,	ZW,	ΑM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM		
	RW:	GH, G	M, KE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,
		DE, D	K, ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,
		BJ, C	F, CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG		
PRAI US 2000-214616P 20000628 GI																

Compds. represented by formula HET-COCR3R4-NX4-CO(CR6R7)m-D [I; wherein m AB = 0, 1 or 2; HET = heterocyclyl; R3, R4 = H,, C1-8 alkyl, CH(R8)-aryl, -CH(R8)-heteroaryl, -CO-3 alkyl-C3-8 cycloalkyl (wherein the aryl or heteroaryl groups are optionally substituted by one or two groups; R8 = H, C1-8 alkyl, -C0-3 alkylaryl, -C0-3 alkylheteroaryl, -C3-6 cycloalkyl); R6, R7 = H, C1-6 alkyl, -C0-3 alkyl-aryl, -C0-3 alkyl-heteroaryl, -C0-3alkyl-C3-8 cycloalkyl; or R6 and R7 together with the nitrogen atom to which they are attached form a 5- or 6-membered ring optionally contg. an addnl. heteroatom selected from O, S, NR3; D = -C0-6 alkylamino-C(:NR7)-NR15R16, -C0-6 alkylaminopyridyl, -C0-6 alkylaminoimidazolyl, -C0-6 alkylaminothiazolyl, -CO-6 alkylaminopyrimidinyl, -CO-6 alkylaminopiperazinyl-R15, -C0-6 alkylmorpholinyl, etc. (wherein R15, R16 = H, -C1-6 alkyl, -C0-3 alkylaryl, -C0-3 alkylheteroaryl, or -C0-3alkyl-C3-8 cycloalkyl, wherein the alkyl and aryl groups are optionally substituted with one or two groups); X4 = H or C1-6 alkyl or X4 is taken together with R4 and the nitrogen atom to which X4 is attached and the carbon atom to which R4 is attached and form a five to seven membered ring] are prepd. Melanocortins are peptides derived from pro-opiomelanocortins (POMC) that bind to and activate G-protein coupled receptors (GPCR's) of the melanocortin receptor family and regulate a diverse no. of physiol. processes including food intake., metab., and thermogenesis as well as sexual dysfunction. These compds. I are useful for the treatment or prevention of disorders, diseases, or conditions  $\frac{1}{2}$ responsive to the activation of melanocortin receptor including obesity, diabetes mellitus, male or female sexual dysfunction, erectile dysfunction, or disorders that cause redn. in appetite, or feeding behavior and/or body wt.; for modulating appetite and metabolic rates; for acutely stimulating the appetite for the treatment of hepatic lipidosis, cachexia, and other pathologies resulting in/from inappropriate food intake and wt. loss; for acutely stimulating the appetite of livestock for the treatment of ketosis, postpartum anestrus, and other metabolic and reproductive pathologies resulting in/from inappropriate food intake and wt. loss; and for enhancing growth and survivability of neonates in livestock. Thus, esterification of N-Boc-L-Tic-OH with N-hydroxysuccinimide using Et3N and EDC in CH2Cl2 at room temp. for 4 h gave 3,4-Dihydro-1H-isoquinoline-2,3-(S)-dicarboxylic acid 2-tert-Bu ester 3-(2,5-dioxopyrrolidin-1-yl) ester which was condensed with D-p-chlorophenylalanine in the presence of Et3N in CH2Cl2 at room temp. overnight to give 3-(S)-[(R)-1-Carboxy-2-(4-chlorophenyl)ethylcarbamoyl]-3,4-dihydro-1H-isoquinoline-2-carboxylic acid tert-Bu ester. The latter compd. was further condensed with 8a-(Pyridin-2-ylmethyl)-2-(2,2,2trifluoroethyl)tetrahydroimidazo[1,5-a]pyrazine-1,3-dione using Et3N and EDC in CH2Cl2 at 0.degree. for 5 h to give (S)-3-[(R)-1-(4-Chlorobenzyl)-2-[1,3-dioxo-8a-(pyridin-2-ylmethyl)-2-(2,2,2-trifluoroethyl) hexahydroimidaz o[1,5-a]pyrazin-7-y1]-2-oxoethylcarbamoy1]-3,4-dihydro-1H-isoquinoline-2carboxylic acid tert-Bu ester which was treated with a mixt. of EtOH and concd. HCl at 0.degree. for 0.5 h to give (S)-1,2,3,4-Tetrahydroisoquinoline-3-carboxylic acid N-[(R)-1-(4-chlorobenzyl)-2-[1,3- $\verb|dioxo-8a-(pyridin-2-y| methyl)-2-(2,2,2-trifluoroethyl)| hexahydroimidazo[1,5-trifluoroethyl]| dioxo-8a-(pyridin-2-y| methyl)-2-(2,2,2-trifluoroethyl)| dioxo-8a-(pyridin-2-y| methyl)| dioxo-8a-(pyridin-2-y| methyl)| dioxo-8a-(pyridin-2-y| methyl)| dioxo-8a-(pyridin-2-y| methylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloophylloop$ a]pyrazin-7-yl]-2-oxoethyl]amide (II) hydrochloride which may be considered as a dipeptide analog hepterocycle amide, N-[N-(L-1,2,3,4-Tetrahydroisoquinoline-3-carbonyl)-D-p-chlorophenylalanyl]-1,3-dioxo-8a-(pyridin-2-ylmethyl)-2-(2,2,2-trifluoroethyl)hexahydroimidazo[1,5a]pyrazine.

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 22 OF 25 REGISTRY COPYRIGHT 2002 ACS

RN 378741-76-5 REGISTRY

CN 3-Isoquinolinecarboxamide, N-[(1R)-1-[(4-chlorophenyl)methyl]-2-[2,3,3a,4,6,7-hexahydro-2-methyl-3-oxo-3a-(phenylmethyl)-5H-pyrazolo[4,3-c]pyridin-5-yl]-2-oxoethyl]-1,2,3,4-tetrahydro-, (3R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C33 H34 C1 N5 O3

CI COM

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 1 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 136:15253 CA

```
ΤI
     Melanocortin receptor agonists, and preparation thereof, for therapeutic
     Bakshi, Raman Kumar; Nargund, Ravi P.; Ye, Zhixiong
IN
     Merck & Co., Inc., USA
PA
SO
     PCT Int. Appl., 59 pp.
     CODEN: PIXXD2
DΤ
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                      KIND
                            DATE
                                           APPLICATION NO.
                                                            DATE
                      ____
                                           ______
PI
     WO 2001091752
                                           WO 2001-US17014
                      A1
                            20011206
                                                            20010525
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO,
             RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ,
             VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     US 2002004512
                      A1 20020110
                                         US 2001-867309
PRAI US 2000-207918P
                      20000530
GI
```

AB The invention discloses compds. and derivs. thereof which are agonists of the human melanocortin receptor(s) and, in particular, are selective agonists of the human melanocortin-4 receptor (MC-4R). They are therefore useful for the treatment, control, or prevention of diseases and disorders responsive to the activation of MC-4R, e.g. obesity, diabetes, sexual dysfunction, including erectile dysfunction and female sexual dysfunction. Prepn. of e.g. I is described.

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

# => d 23 25 sub bib abs

- L5 ANSWER 23 OF 25 REGISTRY COPYRIGHT 2002 ACS
- RN 176714-38-8 REGISTRY

STEREOSEARCH FS

MF C31 H38 N4 O4

SR

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

## REFERENCE 1

ΑN 124:333325 CA

ŤΙ Modification of the potent peptide FK888 with unusual amino acids: effects on activity on neurokinin receptors

ΑU Caliendo, Giuseppe; Greco, Giovanni; Grieco, Paolo; Perissutti, Elisa; Santagada, Vincenzo; Calignano, Antonio; Mancuso, Franca; Novellino, Ettore

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SO Farmaco (1996), 51(3), 197-201 CODEN: FRMCE8

DT Journal

LA English

ΑB We report on the synthesis and the pharmacol. properties of a new series of tachykinin antagonists based on the peptide N2-[(4R)-4-hydroxy-1-[(1methyl-1H-indol-3-yl) carbonyl]-L-prolyl]-N-methyl-N-(phenylmethyl)-3-(2naphthyl)-L-alaninamide (FK 888) modified on the (2-naphthyl)-L-alanine and the [(1-methyl-1H-indol-3-yl)carbonyl] moieties. The compds. were tested on guinea pig ileum for NK-1, rat colon for NK-2 and rat portal vein for NK-3 receptors. The two most potent peptides of this series, Boc-Ioc-Hyp-Phg-NMeBzl (Ioc = (S)-indoline-2-carboxylic acid; Phg = phenylglycine) and Boc-Tic-Hyp-Aoc-NMeBzl (Tic = 1,2,3,4tetrahydroisoquinoline-3-carboxylic acid; Aoc = (S,S,S)-2azabicyclo[3.3.0]octane-3-carboxylic acid), were selective for the NK-2 receptor (pA2 = 7.5 and 7.3, resp.).

- L5 ANSWER 25 OF 25 REGISTRY COPYRIGHT 2002 ACS
- 176177-87-0 REGISTRY RN
- CN L-Arginine, N-[(1,2,3,4-tetrahydro-3-isoquinolinyl)carbonyl]-L-seryl-D-1,2,3,4-tetrahydro-3-isoquinolinecarbonyl-L-(2.alpha.,3a.beta.,7a.beta.)octahydro-1H-indole-2-carbonyl-, (R)- (9CI) (CA INDEX NAME)
- FS PROTEIN SEQUENCE; STEREOSEARCH
- C38 H50 N8 O7 MF
- SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

## REFERENCE 1

AN 124:306933 CA

TI Design and Synthesis of New Linear and Cyclic Bradykinin Antagonists

AU Thurieau, Christophe; Feletou, Michel; Hennig, Philippe; Raimbaud, Eric; Canet, Emmanuel; Fauchere, Jean-Luc

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SO J. Med. Chem. (1996), 39(10), 2095-101 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

AB The synthesis and pharmacol. properties of a new series of small linear and cyclic peptides derived from the 5 C-terminal amino acid residues of second-generation bradykinin receptor antagonists. Variations of the 2 first residues of the pentapeptide (Thi-Ser-D-Tic-Oic-Arg) modulated the biol. activities of the analogs on bradykinin-induced smooth muscle contractions in rabbit jugular vein (RJV), a tissue prepn. specific of the B2 bradykinin receptor. Several analogs showed pA2 values around 7 on this tissue prepn., and 1 cyclic compd., c[-Gly-Thi-D-Tic-Oic-Arg-], in which Thi-Ser was replaced by Gly-Thi, displayed a pA2 of 7.4 on RJV. On the basis of these results, 3 cyclic mols. and their linear counterparts were tested on human umbilical vein, a tissue specific of the human B2 receptor. The pKB values obtained for these compds. on these tissue prepns. were equiv. to those obtained for the decapeptide NPC 567 (4.8 <pA2 < 5.1). NMR and mol. modeling studies performed on 1 of the compds. clearly demonstrated a type II' .beta.-turn structure. This analog may serve as a new lead for the design of nonpeptide ligands of the bradykinin B2 receptor subtype.

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